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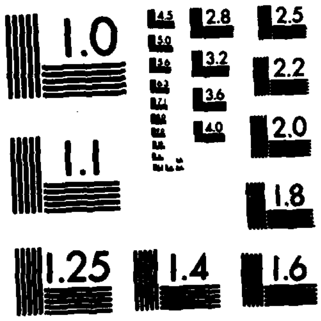

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Methods are developed to represent an acoustic pressure field by a linear combination of modal solutions to the wave equation using a vertical, equally-spaced hydrophone array that may not span the entire water column. Techniques are developed to determine which of the (presumed known) modal functions are present in the representation and to determine the coefficient of each.

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CONTENTS

PILOT EFFORT TO DEFINE IMPROVED NUMERICAL ANALYSIS METHODS FOR THE HANDLING OF MODERATE APERTURE ACOUSTIC ARRAY DATA

Background

The Code 5120 research project "High Resolution of Complex Acoustic Fields Using Moderate Apertures" will, if successful, enhance the operational Navy's ability to detect and track submarines in shallow water or Arctic environments. Initially the project is considering the following physical circumstances: high signal to noise ratio; shallow water (300 meters maximum); a short array of hydrophones (less than 300 meters); and a small number of hydrophones (up to 64).

As part of this initial effort numerical analysis and processing techniques were to be developed. These methods may then be incorporated into experiments as part of the signal processing portion of the experimental apparatus. Thus, successful research should provide numerical-experimental methods to better represent an incident sound pressure field everywhere along an array of hydrophones, the major source of that field initially being controlled by the experimenter.

(Underlying the numerical analysis efforts is the assumption that we will ultimately be involved in a "bootstrapping" operation. That is, a mathematical model derived from the experimental data will be useful for improving the collection and reduction of experimental data; in turn these new data serve as the basis for further analysis and refinement of the mathematical model, and so on.)

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The experiments will probably involve placing sound sources with specifically designed sonic characteristics in the water at preselected points. The mathematics utilized in the signal processing equipment depends upon the results of the research in numerical processing techniques.

In submarine detection and tracking successful techniques would also have to deal with a low signal-to-noise ratio. It is hoped the methods developed in this project will shed light on techniques for use in such noisy environments.

To initiate the development of the numerical and processing techniques, a short term (approximately 2 month) investigation was undertaken by Charles Osgood in collaboration with Richard Heitmeyer and William Moseley.

This investigation made use of the following assumptions:

o The sound pressure field $f(z)$ can be well represented by a linear combination of a few modal solutions to the wave equation;

o The modal solutions are known well numerically (even if not analytically);

o The eigenvalues k_n are also known well numerically;

o Each pressure field is well approximated by a linear combination of, say, the 100 lowest modals;

o Only approximately 20 modals are ever needed to represent any particular pressure field; and,

o The signal-to-noise ratio is high, but some noise is always present.

Introduction

This paper presents for consideration a number of approaches for attacking the problem above which were developed over a ten week period. It is hoped that further research in this area will be aided by the ideas presented.

A few words about the organization of this paper: Section I addresses the problem of determining those modals $u_n(z)$ actually present in the representation of the incident sound pressure field $f(z)$. Section II treats the problem of determining the coefficients of these modal functions $u_n(z)$. There are five appendices expanding on different points. The levels of the different appendices vary from being more tutorial than the main text to being more technical than the main text.

Section I

Let $f(z)$ denote the incident pressure field on the water column where measurements are being made. Let H denote the depth of the water. Let the z_j, $1 \leq j \leq N$, denote the assumed depths of the N hydrophones. As it happens, we shall always assume that the hydrophones are equally spaced, so let $h = z_{j+1} - z_j$. It is assumed that the emitter has a constant frequency ω. Let $c(z)$ denote the speed of sound at depth z in a neighborhood of the water column.

From [2] we know that in shallow water we may assume that

$$f(z) = \Sigma_n A_n u_n(z)$$

where each modal function satisfies a differential equation of the form

$$\left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_n^2\right) u_n(z) = 0$$

for some constant k_n.

Determining the k_n's of the modals involved in representing a particular $f(z)$ is the problem now considered. Let $\psi = \dfrac{d^2}{dz^2} - \dfrac{\omega^2}{c^2(z)}$. It is shown in Appendix I that if d modals are needed to represent $f(z)$ then for almost all choices of equally spaced $z_1,\ldots,z_d$ the polynomial equation in y

$$\begin{vmatrix} 1 & f(z_1) & \cdots & f(z_d) \\ y & \psi f(z_1) & \cdots & \psi f(z_d) \\ \vdots & \vdots & & \vdots \\ y^d & \psi^d f(z_1) & \cdots & \psi^d f(z_d) \end{vmatrix} = 0 \qquad (1)$$

will not vanish identically and will have as roots exactly those $(-k_n^2)$ corresponding to the d modals $u_n(z)$ needed to represent $f(z)$. (If fewer than d modals are needed then the polynomial in (1) vanishes identically.)

Obviously in trying to use (1) there is (probably well founded) concern about approximating high order derivatives numerically. One should calculate the polynomial in (1) with t replacing d for $t = 1,2,\cdots$, until a zero polynomial is obtained. Then backing up to a d+1 by d+1 matrix, the roots of (1) should be determined. Error in approximating the $\psi^{\ell}f(z_j)$ could even make it impossible to tell which polynomial equation to solve. (On the other hand, if the values of the $\psi^{\ell}f(z_j)$ have been accurately determined "solved" is too strong a word to describe the necessary calculations. The roots must be included among a set of no more than 100 numbers; therefore, the polynomial need only be evaluated 100 times.)

A variant of the above idea is discussed in Appendix II. It seems more likely that differences of the form $f(z+h)-f(z)$ can be more accurately obtained than can derivatives of $f(z)$. The difficulty with this observation is that we seem to have only a differential equation available for use. In a very important case, however, we do have difference equations which are satisfied by the modal functions.

In the case of constant sound speed (in the water column) we obtain solutions of the form $u_n(z) = \sin(\theta_n z)$. [More correctly $u_n(z)$ is proportional to $\sin(\theta_n z)$ but we shall ignore that point in this paper.] Second it is "folklore" in the field that in cases of actual interest the higher subscripted modals look as if they are sin's. In Appendix III it is shown that if one replaces ψ throughout equation (1) by the operator ψ_h where $\psi_h g(z) = g(z+h)-2g(z)+g(z-h)$ then the polynomial equation replacing (1) has roots equal to the numbers $-(2\sin(\theta_n \frac{1}{2}h))^2$. [Since we do not divide by h^2 the noise is less likely to be exaggerated. Note that $h^{-2}\psi_h \to \frac{d^2}{dz^2}$ as $h \to 0$ and that $-h^{-2}(2\sin\theta_n \frac{1}{2}h)^2 \to \theta_n^2$ as $h \to 0$.]

What about the lower subscripted modals, in the situation where the higher subscripted modals look sinusoidal? Let $u_n(z)$ be one of the higher subscripted modals which is supposed to look like $\sin \theta_n z$ for some θ_n. Since

$$\frac{d^2}{dz^2} \sin \theta_n z = -\theta_n^2 \sin \theta_n z \quad \text{and}$$

$$\frac{d^2}{dz^2} u_n(z) \left(\frac{\omega^2}{c^2(z)} - k_n^2 \right) u_n(z)$$

we conclude that

$$\frac{\omega^2}{c^2(z)} - k_n^2 \cong -\theta_n^2 .$$

This approximation is probably less good than the original approximation $u_n(z) \cong \sin \theta_n z$. We, therefore, draw only the weak (and heuristic) conclusion from this that $c(z)$ varies slowly. It should then follow that the lower subscripted modals look, locally, like $\sin(\phi_n + \theta_n z)$, for constants θ_n and ϕ_n. [The general solution of $y'' = -\theta_n^2 y$ is of the form $A_n \sin(\phi_n + \theta_n z)$]. Therefore, if the hydrophones are on a small enough interval, we would expect the above polynomial equation to have roots $-(2 \sin (\theta_n \frac{1}{2} h))^2$ corresponding to lower subscripted modals which are (locally) proportional to $\sin (\phi_n + \theta_n z)$.

That is, we would expect to obtain these numbers as roots except for noise in the measured values of $f(z)$. Ideally we would like to smooth the data rather than differencing it. In a sense it is possible to accomplish our desire by using some mathematical trickery applied to the above (difference) method of calculating the roots $-(2 \sin (\theta_n \frac{1}{2} h))^2$.

In Appendix III it is shown how we may construct $F_k(z)$, a linear combination of the functions $f(z)$, $f(z-h)$, $f(z-2h)$,..., with positive coefficients, which when differenced still stays a linear combination of the $f(z)$, $f(z-h)$, $f(z-2h)$,..., with positive coefficients. Further, one can use the set of $F_k(z)$'s (there is one for $k = 0,1,\ldots$) to construct a polynomial equation

from whose roots the θ_n can be determined. (On the other hand, this method does require more data points than do the methods discussed previously; additionally, the degree of the polynomial equation doubles from d to 2d).

Trying to verify the locations of roots to these polynomial equations may prove difficult. A probably much better method of root verificiation applies to the polynomial equation obtained in Appendix III ((2) below) as well as to a modified version of equation (1) ((3) below); this method is discussed next.

The equation obtained in Appendix III is of the form

$$\begin{vmatrix} 1 & F_0(z_\ell) & F_1(z_\ell) & \cdots & F_{2d-1}(z_\ell) \\ y & F_1(z_\ell) & F_2(z_\ell) & & F_{2d}(z_\ell) \\ \vdots & \vdots & \vdots & & \vdots \\ y^{2d} & F_{2d}(z_\ell) & F_{2d+1}(z_\ell) & \cdots & F_{4d-1}(z_\ell) \end{vmatrix} = 0 \qquad (2)$$

One could have obtained an analogue of equation (1) of the form

$$\begin{vmatrix} 1 & f(z_d) & \psi f(z_d) & \cdots & \psi^{d-1} f(z_d) \\ y & \psi f(z_d) & \psi^2 f(z_d) & \cdots & \psi^{d} f(z_d) \\ \vdots & \vdots & \vdots & & \vdots \\ y^{d} & \psi^d f(z_d) & \psi^{d+1} f(z_d) & \cdots & \psi^{2d-1} f(zd) \end{vmatrix} = 0 \qquad (3)$$

which has the same roots as equation (1). [If ψ_h substitutes for ψ, (3) has the roots $-(2\sin(\theta_n \frac{1}{2} h))^2$ if the modals are sinusoidal. Note (3) needs more data points than does (1).]

Form the polynomials

$$\sum_{j=0}^{2d-1} (\psi^j f(z_d)) x^j \quad \text{and} \quad \sum_{j=0}^{4d-1} F_j(z_\ell)\, x^j,$$

respectively. Consider the problem of approximating these respective polynomials by rational functions. There always exist polynomials u_1, v_1, u_2, and v_2 of degrees not exceeding d-1, d, 2d-1, and 2d, respectively, such that:

$$u_1 v_1^{-1} = \sum_{j=0}^{2d-1} (\psi^j f(z_d))x^j$$

plus terms of higher degree in x

and

$$u_2 v_2^{-1} = \sum_{j=0}^{4d-1} F_j(z_\ell)x^j$$

plus terms of higher degree in x. Almost always (in a sense which could be made mathematically precise) u_1, v_1, u_2, and v_2 are of degrees exactly d-1, d, 2d-1, and 2d. Further these polynomials are unique (if we demand their leading coefficient be one) and the zeros of v_1 and v_2 are, respectively, the reciprocals of the roots of (3) and the reciprocals of the roots of (2).

As is explained in Appendix IV there is an efficient algorithm to calculate values of the rational functions $u_1\ v_1^{-1}$ and $u_2\ v_2^{-1}$. If we are at a pole (infinity) of the rational function we have determined a root of the associated equation.

The residues of these rational functions at their poles can be related to the coefficients of the modals in their representation of f(z). For example, the residue of $u_1\ v_1^{-1}$ at $z = -k_n^2$ is $-A_n k_n^{-2}$. Therefore $\lim_{z \to -k_n^2} (z + k_n^{-2})\ u_1\ v_1^{-1} = -A_n\ k_n^{-2}$. It might or might not be reasonable to compute the A_n this way. In any event this brings us to consideration of ways of calculating the A_n.

Section II

Finding the A_n's can be approached in several ways depending upon what assumptions are made. In the general case we have that

$$\left(\prod_{j\neq n}\left(\frac{d^2}{dz^2}-\frac{\omega^2}{c^2(z)}+k_j^2\right)\right)f(z) = \left(\prod_{j\neq n}\left(k_j^2-k_n^2\right)\right)A_n u_n(z). \tag{4}$$

[For a more gradual introduction to the use of products of differential operators see Appendix V.]

Because of the difficulty of computing derivatives numerically, this may not be a feasible way of finding the A_n. As in Section I, it seems reasonable to utilize the operator ψ_h. Then we can write

$$\left(\prod_{j\neq n}\left(\psi_h+\left(2\sin\ \theta_j\frac{h}{2}\right)^2\right)\right)f(z_{d-1}) =$$

$$\left(\prod_{j\neq n}\left(\left(2\sin\ \theta_j\frac{h}{2}\right)^2-\left(2\sin\ \theta_n\frac{h}{2}\right)^2\right)\right)A_n u_n(z_{d-1}).$$

This expression should be valid whenever each $u_n(z) \cong \sin(\phi_n + \theta_n z)$. (Something like this idea should work in the situation of Appendix III where f(z) is replaced by a linear combination of f(z), f(z-h),... having positive coefficients. The exact algebra would be different however.)

There is another approach, however, which is what will be discussed next. [In Appendix V more detail is provided.] Set $x = \pi(z-z_1)(z_N-z_1)^{-1}$ and let k denote a non-negative integer. Suppose one multiplies both sides of (4) by $(\sin\pi x)^{2d-2+k}\ u_n(z)$ and integrates the resultant expression over $[z_1,z_N]$. Because of the high order of vanishing of the integrands at $z = z_1$ and $z = z_N$ it is possible to use integration by parts 2(d-1) times on the left hand integral and, finally, obtain an integrand there which is free of derivatives of f(z). This integral looks like

$$\int_{z_1}^{z_N} f(z) \left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_j^2 \right) \right] (\sin x)^{2d-2+k} \; u_n(z) \; dz. \qquad (5)$$

At least the 2d-2 power of sin πx is mandated by the requirement that we perform 2d-2 integrations by parts without having derivatives of f(z) appear. The reason for possibly wishing that $k > 0$ is that then the integrand in (5) will agree (in value and derivatives) up to the order k at $z = z_1$ and at $z = z_N$. Since (5) must be evaluated by numerical integration we are interested in the rate of convergence of some types of numerical integration schemes. Having the integrand agree to a high order at the two points $z = z_1$ and $z = z_N$ can be expected to add considerable accuracy in the numerical integration. (See Appendix V for details.)

Appendix V discusses approaches to evaluating

$$\left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_j^2 \right) \right] (\sin x)^{2d-2+k} \; u_n(z)$$

quickly using the Fast Fourier Transform.

Appendix I

A possible way to determine the k_n's corresponding to the modal function $u_n(z)$ involved in $f(z)$ is the following:

Write

$$f(z) = \Sigma_n A_n u_n(z)$$

where the $u_n(z)$ are the d modal functions appearing in the decomposition of $f(z)$. Suppose that one can determine good numerical approximations to

$$f(z), \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)}\right) f(z), \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)}\right)^2 f(z), \ldots, \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)}\right)^d f(z)$$

for the d different points z_1, $z_2 = z_1 + h, \ldots, z_d = z_1 + (d-1)h$. At each point z_j the values of the different $\left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)}\right)^i f(z_j)$ are of the form $\Sigma_n A_n (-k_n^2)^i u_n(z_j)$.

For simplicity resubscript the d modals so they are denoted as $u_1(z), \ldots, u_d(z)$. Since the $-k_n^2$ are distinct numbers the determinant of the matrix

$$A = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ -k_1^2 & -k_2^2 & & -k_d^2 \\ \vdots & \vdots & & \vdots \\ (-k_1^2)^{d-1} & (-k_2^2)^{d-1} & \cdots & (-k_d^2)^{d-1} \end{pmatrix} = ((-k_n^2)^{i-1})$$

does not vanish. (This is by the nonvanishing of the Vandermonde determinant.)

Let

$$B = \begin{pmatrix} A_1 u_1 (z_1) & A_1 u_1 (z_2) & \cdots & A_1 u_1 (z_d) \\ A_2 u_2 (z_1) & A_2 u_2 (z_2) & & A_2 u_2 (d_d) \\ \vdots & \vdots & & \vdots \\ A_d u_d (z_1) & A_d u_d (z_2) & \cdots & A_d u_d (z_d) \end{pmatrix} = (A_n u_n (z_j)).$$

If B is nonsingular then so is the matrix

$$AB = \left(\left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)}\right)^{\ell} f(z_j)\right)$$

where $1 \leq \ell + 1 \leq d$ and $1 \leq j \leq d$.

Since by hypthesis $A_1A_2 \ldots A_d \neq 0$, the nonsingularity of B is equivalent to the nonsingularity of the matrix $(u_n(z_j))$. Assume the u_n are analytic functions. Then $|u_n(z_1 + (j-1)\, h)| = M(z_1,h)$ is an analytic function of h. For each fixed z_1, if $M(z_1,h)$ vanishes for an infinite number of h, $0 \leq h \leq H$, then $M(z_1,h) \equiv 0$, for this value of z_1, as a function of h. Define Δ_h by $\Delta_h\, g(z) = (g(z+h) - g(z))h^{-1}$.

There exist constants e_{jl}, depending upon h but independent of n such that:

$$\begin{pmatrix} u_1(z_1) & \Delta_h u_1(z_1) & \cdots & \Delta_h^{d-1} u_1(z_1) \\ u_2(z_1) & \Delta_h u_2(z_1) & \cdots & \Delta_h^{d-1} u_2(z_1) \\ \vdots & \vdots & & \vdots \\ u_d(z^1) & \Delta_h u_d(z_1) & \cdots & \Delta_h^{d-1} u_d(z_1) \end{pmatrix} \begin{pmatrix} e_{11} \cdots e_{1d} \\ \vdots \quad \vdots \\ e_{d1} \cdots e_{dd} \end{pmatrix} = \begin{pmatrix} u_1(z_1) & \cdots & u_1(z_d) \\ \vdots & & \vdots \\ u_d(z_1) & \cdots & u_d(z_d) \end{pmatrix};$$

hence, $M(z_1,h) = N(h)|(\Delta_h)^{\ell} u_n(z_1)|$. Since

$$\begin{pmatrix} e_{11} & \cdots & e_{1d} \\ \vdots & & \vdots \\ e_{d,1} & \cdots & e_{dd} \end{pmatrix}$$

is nonsingular if $h \neq 0$, it follows that $N(h) \not\equiv 0$.

Suppose that $M(z_1,h) \equiv 0$. Taking the limit as $h \to 0$, $|\Delta_h^{\ell}\, u_n(z_1)|$ becomes $|u_n^{(\ell)}(z_1)|$, the Wronskian of $u_1, \ldots, u_n$ evaluated at $z = z_i$.

The Wronskian of a set of linearly independent analytic functions cannot vanish identically. Thus, except for at most a finite set of values of z_1,

$$\begin{vmatrix} u_1(z_1) & \cdots & u_1(z_d) \\ \vdots & & \vdots \\ u_d(z_1) & \cdots & u_d(z_d) \end{vmatrix} = 0$$

for at most a finite set of values of h.

Therefore, in practice, for almost all pairs (z_1,h), $|u_n(z_j)| \neq 0$, and B is nonsingular. When B is nonsingular we have, where $\psi = \dfrac{d^2}{dz^2} - \dfrac{\omega^2}{c^2(z)}$,

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ -k_1^2 & -k_2^2 & \cdots & (-k_d^2) \\ \vdots & & & \vdots \\ (-k_1^2)^d & (-k_2^2)^d & \cdots & (-k_d^2)^d \end{pmatrix} = \begin{pmatrix} f(z_1) & f(z_2) & \cdots & f(z_d) \\ \psi f(z_1) & \psi f(z_2) & \cdots & \psi f(z_d) \\ \vdots & \vdots & \vdots & \vdots \\ \psi^d f(z_1) & \psi^d f(z_2) & \cdots & \psi^d f(z_d) \end{pmatrix} B^{-1}.$$

(Notice that both of the matrices which have been written out have dimension $d + 1$ by d while B^{-1} has dimensions d by d.) This implies that each $d + 1$ by 1 column vector

$$\begin{pmatrix} 1 \\ -k_n^2 \\ \vdots \\ (-k_n^2)^d \end{pmatrix}$$ can be written as a linear combination

of the d different d + 1 by 1 column

vectors $\begin{pmatrix} f(z_j) \\ \psi f(z_j) \\ \cdot \\ \cdot \\ \cdot \\ \psi^d f(z_j) \end{pmatrix}$.

Therefore

$$\begin{vmatrix} 1 & f(z_1) & \cdots & f(z_d) \\ y & \psi f(z_1) & \cdots & \psi f(z_d) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ y^d & \psi^d f(z_1) & \cdots & \psi^d f(z_d) \end{vmatrix} = 0$$

has exactly the roots $y = -k_j^2$.

Appendix II

We shall derive an alternative to the equation obtained in Appendix I, under the conditions that each

$$u_n(z) \simeq \sin(\phi_n + \theta_n z)$$

for constants ϕ_n and θ_n. As an approximation to $\frac{d^2}{dz^2}$ we use $h^{-2}\psi_h$ where

$h^{-2}\psi_h g(z) = h^{-2}(g(z+h) - 2g(z) + g(z-h))$.

Then $h^{-2}\psi_h e^{i\theta_n z} = h^{-2}\left(e^{i\theta_n h} - 2 + e^{-i\theta_n h}\right)e^{i\theta_n z}$

$$= -h^{-2}\left(\frac{e^{\frac{1}{2}i\theta_n h} - e^{-\frac{1}{2}i\theta_n h}}{i}\right)^2\left(e^{\frac{1}{2}i\theta_n z}\right)^2 = -\left(\frac{\sin\frac{1}{2}\theta_n h}{\frac{1}{2}h}\right)^2 \theta^{i\theta_n z}.$$

(As a check, if $h \to 0$ we obtain $-\theta_n^2 e^{i\theta_n z}$ which agrees with $\frac{d^2}{dz^2} e^{i\theta_n z}$.)

Since we are <u>not</u> going to pass to the limit, we discard the h^{-2} factor and shall only use ψ_h in what follows. Writing

$$\sin(\theta_n + \theta_n z) = \frac{1}{2i}\left(e^{i(\phi_n + \theta_n z)} - e^{-i(\phi_n + \theta_n z)}\right)$$

we see that

$\psi_h \sin(\phi_n + \theta_n z) = -(2\sin(\phi_n \frac{1}{2}h)^2 \sin(\phi_n + \theta_n z)$.

The exact form of the operation $\psi = \frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)}$ used in Appendix I was irrelevant to the argument there leading to the polynomial equation for the $-k_n^2$. What was important was that the operator used had the $u_n(z)$ as eigenfunctions (and that the eigenvalues were distinct). Thus we conclude that if h is chosen so that the $(\sin\theta_n \frac{1}{2}h))^2$ are distinct, then

$$\begin{vmatrix} 1 & f(z_1) & \cdots & f(z_d) \\ y & \psi_h f(z_1) & \cdots & \psi_n f(z_d) \\ \vdots & \vdots & & \vdots \\ y^d & \psi_h^d f(z) & \cdots & \psi_h^d f(z_d) \end{vmatrix} = 0$$

has as its roots exactly the $-(2\sin|\theta_n \frac{1}{2}h)^2$.

Appendix III

As before it is assumed that $f(z)$ has been measured at equally spaced points $z_1,\dots,z_N$ with $z_{j+1} - z_j = h$. Next below define $f(z)$ to vanish identically if $z < z_1$.

Let $r > 1$. For $k = 1,2,\dots,$ and $1 \le \ell \le N$, set

$$F_k(z_\ell) = \sum_{j=0}^{\infty} \binom{k+j-1}{j} r^{-j} f(z_{\ell-k-j}).$$

Notice that

$$F_k(z_{\ell+1}) - r^{-1}F_k(z\ ) =$$

$$\left(\sum_{j=0}^{\infty}\left[\binom{k+j}{j+1} - \binom{k+j-1}{j}\right] r^{-j-1} f(z_{\ell-i-j})\right) + f(z_{\ell+1-k})$$

$$= \left(\sum_{j=0}^{\infty} \binom{k-1+j}{j+1} f(z_{-(k-1)-(j+1)}) r^{-j-1}\right) + f(z_{\ell+1-k}),$$

which equals $f(z_\ell)$ if $k = 1$, but which otherwise is equal to

$$\sum_{j=0}^{\infty} \binom{k-1+j-1}{j} f(z_{\ell-(k-1)-j}) r^{-j} = F_{k-1}(z_\ell).$$

Setting $F_o(z_\ell) = f(z_\ell)$ we have that if $k \ge 1$, $F_k(z_{\ell+1}) - r^{-1}F_k(z_\ell) = F_{k-1}(z_\ell)$.

The idea is to choose r sufficiently large that $\binom{k+j-1}{j} r^{-j}$ is quite small whenever $\ell - k - j \le 0$. Then each $F_k(z_\ell)$ will "almost" be the same as the value which would have been obtained from using the (unknown) representation of $f(z)$ as $\sum_n A_n \sin(\phi_n + \theta_n z)$ to define $f(z)$ for $z = z_o, z_{-1}, \cdots$.

Notice that $\displaystyle\sum_{j=0}^{\infty} \binom{k+j-1}{j} r^{-j} e^{\,i(\phi_n + \theta_n z_{\ell-(j+k)})}$

$$= \left(\sum_{j=0}^{\infty} \binom{k+j-1}{j} r^{-j} e^{-i(\theta_n (j+k) h)}\right) e^{i(\phi_n + \theta_n z)}$$

$$= r^k (re^{i\theta_n h} - 1)^{-k}\, e^{i(\phi_n + \theta_n z)}.$$

Setting each $r(re^{i\theta_n h}-1)^{-1} = R_n \exp(i\Phi_n)$, every $F_k(z_\ell) \cong \sum_n A_n R_n^k \sin(\Phi_n + k\,\Phi_n + \theta_n z_\ell)$.

At this stage not knowing the θ_n's and ϕ_n's [which are what we wish to determine] all we can really use of the above formula is that each $F_k(z_\ell)$ is a linear combination of 2d exponentials.

By an argument quite similar to that in Appendix I, but with the 2d exponentials here replacing the d sinusoidal functions there, we see that the roots of the polynomial equation

$$\begin{vmatrix} 1 & F_0(z_\ell) & \cdots & F_{2d-1}(z_\ell) \\ y & F_1(z_\ell) & \cdots & F_{2d}(z_\ell) \\ \vdots & \vdots & & \vdots \\ y^{2d} & F_{2d}(z_\ell) & \cdots & F_{4d-1}(z_\ell) \end{vmatrix} = 0$$

are $y = r(re^{\pm i\theta_n h}-1)^{-1} = R_n^{\pm 1}$.

Appendix IV

There is a mathematical theory of best rational (function) approximation to power series. Assuming a property of $g(x)$ (the power series to be approximated) which is called normality (because it "normally" holds) the following are true:

For each pair of non-negative integers m and n there exist unique monic polynomials $p_{mn}(x)$ and $q_{mn}(x)$ having degrees exactly m and n, respectively, such that $p_{mn}(x)(q_{mn}(x))^{-1}$ agrees with $g(x) = \sum_{J=0}^{\infty} \alpha_j x^J$ in its power series expansion about $x = 0$ through the term $\alpha_{m+n} x^{m+n}$ but no further.

If we consider a polynomial $g_M(x) = \sum_{J=0}^{M} \alpha_j x^j$ its coefficients α_j for $j > M$ are not typical of the class of all power series in x. We do not expect $g_M(x)$ to be normal; however, one expects a random $g_M(x)$ to display the attributes of a normal series, as long as the coefficients of powers of x higher than M are not involved.

The $p_{mn}\ q_{mn}^{-1}$ are known as the Pade' approximation (of $g(x)$ or $g_N(x)$) and they are denoted by r_{mn}, i.e. $r_{mn} = p_{mn}\ q_{mn}^{-1}$. In 1966 Wynn discovered the following new identify relating the r_{mn} for a normal $g(x)$. Wynn showed that $(r_{m+1,n} - r_{m,n})^{-1} + (r_{m-1,n} - r_{m,n})^{-1} = (r_{m,n+1} - r_{m,n})^{-1} + (r_{m,n-1} - r_{m,n})^{-1}$.

We quote from [1]:

"Wynn's identity permits the recursive construction of a normal Pade' table from the partial sums $r_{mo}(x) = C_m(x) = \sum_{j=0}^{m} \alpha_j x^j$ according to the scheme in Table 7.

Table 7

$$
\begin{array}{c|cccccc}
 & 0 & 0 & 0 & 0 & 0 & 0 \;\ldots \\
\hline
\infty & C_0 & r_{01} & r_{02} & r_{03} & r_{04} & \cdots \\
\infty & C_1 & r_{11} & r_{12} & r_{13} & & \\
\infty & C_2 & r_{21} & r_{22} & & & \\
\infty & C_3 & r_{31} & & & & \\
\infty & C_4 & & & & & \\
\infty & \vdots & & & & & \\
\vdots & & & & & &
\end{array}
$$

(Notice that to initialize properly each $r_{m,-1} =$ and each $r_{-1,n} = 0$. The calculation proceeds in the order indicated by the arrows.)

Actually calculating these $r_{m,n}$ as functions might be very difficult unless one possessed symbol manipulation software. On the other hand upon replacing x by *any specific* value x_o in the $r_{m,o} = C_m$ the calculation yields $r_{m,n}(x_o)$.

Appendix V

We assume that the $u_n(z)$ which appear in the modal decomposition of $f(z)$ are known and that each modal satisfies a linear differential equation of the form

$$\left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_n^2\right) u_n(z) = 0.$$

Since the modals are known the set of constants k_n is known; what is unknown is the set of coefficients A_n of the $u_n(z)$ in the representation of $f(z)$.

Suppose for simplicity that modals $u_1, \cdots, u_d$ appear in the representation of f. Then one notes that

$$g_1 = \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_1^2\right) f(z)$$

$$= \sum_{n=1}^{d} (k_1^2 - k_n^2) A_n u_n (z)$$

$$= \sum_{n=2}^{d} (k_1^2 - k_n^2) A_n u_n(z).$$

Applying $\left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_2^2\right)$ to $g_1(z)$ yields

$$g_2(z) = \sum_{n=3}^{d} \left(k_1^2 - k_n^2\right)\left(k_2^2 - k_n^2\right) A_n u_n(z).$$

Continuing,

$$g_{d-1} = \left[\prod_{n=1}^{d-1} \left(\left(\frac{d}{dz}\right)^2 - \frac{\omega^2}{c^2(z)} + k_n^2\right)\right] f(z)$$

$$= \left[\prod_{n=1}^{d-1} \left(k_n^2 - k_d^2\right)\right] A_d u_d(z).$$

Generalizing,

$$\left[\prod_{j\neq n}\left(k_j^2 - k_n^2\right)\right] A_j\, u_j(z) = \prod_{j\neq n}\left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_j^2\right) f(z),$$

for $n = 1,2,\cdots,d$.

One might well worry about calculating derivatives of f numerically up to the order $2d-2$, if d is any size. One possible way out is the following approach:

Set $x = \pi(z-z_1)(z_N-z_1)^{-1}$. Notice that the equation

$$g_1 = \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_1^2\right) f(z)$$

implies, by multiple use of integration by parts, that

$$\int_{z_1}^{z_N} g_1(z)\sin^2 x\, dz = \int_{z_1}^{z_N}\left[\left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_1^2\right) f(z)\right]\sin^2 x\, dz$$

$$= \int_{z_1}^{z_N}\left(\left(\frac{d}{dz}\right)^2 f(z)\right)\sin^2 x\, dz + \int_{z_1}^{z_N} f(z)\left(\frac{-\omega^2}{c^2(z)} + k_1^2\right)\sin^2 x\, dx$$

$$= -\int_{z_1}^{z_N} f^{(1)}(z)\,\frac{d}{dz}(\sin^2 x)\, dx + \int_{z_1}^{z_N} f(z)\left(\frac{-\omega^2}{c^2(z)} + k_1^2\right)\sin^2 x\, dx$$

$$= \int_{z_1}^{z_N} f(z)\,\frac{d^2}{dz^2}(\sin^2 x)\, dx + \int_{z_1}^{z_N} f(z)\left(\frac{-\omega^2}{c^2(z)} + k_1^2\right)\sin^2 x\, dx$$

$$= \int_{z_1}^{z_N} f(z)\left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_1^2\right)\sin^2 x\, dx.$$

One see that in, general, if we have d modals in the decomposition of $f(z)$ then

$$\int_{z_1}^{z_N} \left(\left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{2}{c^2(z)} + k_n^2 \right) \right] f(z) \right) \sin^{2d-2} x \, dz$$

$$= \int_{z_1}^{z_N} f(z) \left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_n^2 \right) \right] \sin^{2d-2} x \, dz$$

$$= A_n \int_{z_1}^{z_N} \prod_{j \neq n} \left(k_j^2 - k_n^2 \right) u_n(z) \sin^{2d-2} x \, dz.$$

One hopes that

$$\left| \int_{z_1}^{z_N} u_n(z) \sin^{2d-2} x \, dz \right|$$

is not too small and that A_n can be determined upon using numerical integration to approximate

$$\int_{z_1}^{z_N} f(z) \left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_j^2 \right) \right] \sin^{2d-2} x \, dz$$

from knowledge of the value of the integrand at the points $z_1, z_2, \cdots, z_N$.

With the basic idea of the above derivation in mind, it becomes clear that we did not have to choose $\sin^{2d-2} x$ above as a multiplier. Other possible choices are $\sin^{2d-2} x \; u_n(z)$, $\sin^{2d-2+k} x$ for a positive integer k, or $\sin^{2d-2+k} x \; u_n(x)$, also for a positive integer k. We refer to these possibilities as option one, option two, and option three.

Option one has the good feature that now the coefficient of A_n is an integral having an integrand which always maintains the same sign. Option one has the potential drawback that if $|u_n(z)| < 1$ and $u_n(z)$ does not

change sign on $[z_1, z_N]$ we have not improved our situation. A further drawback is that calculating

$$\left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_j^2\right)\right] \sin^{2d-2} x \, u_n(z)$$

may be much more difficult than calculating the same expression without the $u_n(z)$.

Call the integrand obtained after many integrations by parts $G_k(z)$. Option two forces $G_k^{(j)} = G_k^{(d)}(z_N)$ for $j = 0, 1, \ldots, k-1$. For such integrands the very simple integration formula $\sum_{j=1}^{N-1} G_k(z_j)$ can be expected to be quite good. (One can give an argument as to why this is so which is based on the rate of convergence of the Fourier series for $G_k(z)$ on $[z_1, z_N]$. The coefficients of e^{+2inx} should be smaller in absolute value than a constant, depending on k, times n^{-k}.) This is a good feature of option two; the only obvious bad feature is that the integrand gets somewhat more complicated as k increases. Option three simply combines options one and two.

Suppose that c(z) is slowly varying enough to be well approximated on $[z_1, z_N]$ by a constant and that k is even, say $k = 2k_1$. Then $(\sin^2 x)^{d-1+k_1} = \left(\frac{1}{2} - \frac{\cos 2x}{2}\right)^{d-1+k_1}$, and it appears that the problem of evaluating

$$\left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_j^2\right)\right] (\sin^2 x)^{d-1+k_1} \quad z = z_1, z_2, \cdots, z_N$$

can be carried out inexpensively using the Fast Fourier transform (FFT) on $[z_1, z_N]$.

What about options one and three where one must evaluate

$$\left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_j^2\right)\right] \sin^{2d-2+2k_1} x \, u_n(x),$$

for $k_1 \geq 0$, at $z = z_1, z_2, \cdots, z_N$? This could be difficult without either

software capable of symbol manipulation or more mathematical investigation. One possible trick is the following: suppose positive integers j_1 and j_2 can be found with j_1 only a little larger than one and j_2 only a little smaller than N such that $u_n(z) = \sin(\theta_n z)$ is periodic with a period of (approximately) $z_{d_2} - z_{d_1}$. Then, substituting the interval $[z_{d1}, z_{d2}]$ for $[z_k, z_B]$ above (including in the definition of x), we have that $u_n(z) = \sin 2^{\ell} x$ for some positive integer ℓ. In this case the FFT (but now the FFT on $[z_{d_1}, z_{d_2}]$) can be used to calculate

$$\left[\prod_{j \neq n} \left(\frac{d^2}{dz^2} - \frac{\omega^2}{c^2(z)} + k_j^2\right)\right] \sin^{2d-2+2k_1} x \; u_n(x) \text{ also.}$$

References

[1] W. B. Gragg, The PADE' Table and Its Relation to Certain Algorithms of Numerical Analysis, SIAM Review, vol. 14, No. 1, January 1972 page 1.

[2] John F. MIller and Frank Ingenito, Normal Mode Fortran Programs for Calculating Sound Propagation in the Ocean, NRL Memorandum Report 3071, June 1975.

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